J. Braz. Chem. Soc., Vol. 23, No. 10, S1-S3, 2012.
Printed in Brazil - ©2012 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Supplementary Information

A Simple Method to Evaluate, Correlate and Predict Boiling and Flash Points of Alkynes

Justin M. Godinho,[a] Felix A. Carroll[a] and Frank H. Quina*[,b]

[a]Department of Chemistry, Davidson College, 28035 Davidson, NC, USA

[b]Instituto de Química, Universidade de São Paulo, CP 26077, 05513-970 São Paulo-SP, Brazil

Table S1. Boling point data

entry	compound	Lit. T_B/K	Ref.	Lit. Y_{BP}	A_i	C	M_3	M	D	S	Pred. Y_{BP}	Pred. T_B/K	AD/K
1	1-hexyne	344.48	1	19.15	−0.324	6	0	0	0	1.00	18.65	338.65	5.83
2	3-hexyne	352.94	2	19.90	0.298	6	0	0	0	1.00	19.27	345.87	7.06
3	2-hexyne	357.00	3	20.26	1.261	6	0	0	0	1.00	20.24	356.71	0.29
4	1-heptyne	372.89	1	21.74	−0.324	7	0	0	0	1.00	21.43	369.59	3.30
5	3-heptyne	379.15	4	22.35	0.298	7	0	0	0	1.00	22.05	376.07	3.08
6	2-heptyne	385.15	5	22.95	1.261	7	0	0	0	1.00	23.01	385.83	0.68
7	1-octyne	399.35	1	24.40	−0.324	8	0	0	0	1.00	24.21	397.48	1.87
8	4-octyne	404.70	3	24.97	0.211	8	0	0	0	1.00	24.74	402.55	2.15
9	3-octyne	406.15	5	25.13	0.298	8	0	0	0	1.00	24.83	403.37	2.78
10	2-octyne	411.15	3	25.67	1.261	8	0	0	0	1.00	25.79	412.26	1.11
11	1-nonyne	423.85	6	27.09	−0.324	9	0	0	0	1.00	26.99	422.92	0.93
12	4-nonyne	427.15	5	27.47	0.211	9	0	0	0	1.00	27.52	427.57	0.42
13	3-nonyne	429.82	3	27.78	0.298	9	0	0	0	1.00	27.61	428.32	1.50
14	2-nonyne	435.05	6	28.40	1.261	9	0	0	0	1.00	28.57	436.49	1.44
15	1-decyne	447.15	1	29.87	−0.324	10	0	0	0	1.00	29.77	446.32	0.83
16	4-decyne	450.15	6	30.24	0.211	10	0	0	0	1.00	30.30	450.61	0.46
17	5-decyne	450.15	6	30.24	0.211	10	0	0	0	1.00	30.30	450.61	0.46
18	3-decyne	452.45	6	30.53	0.298	10	0	0	0	1.00	30.39	451.31	1.14
19	2-decyne	457.75	6	31.21	1.261	10	0	0	0	1.00	31.35	458.88	1.13
20	1-undecyne	468.16	6	32.57	−0.324	11	0	0	0	1.00	32.55	468.00	0.16
21	5-undecyne	471.15	6	32.97	0.211	11	0	0	0	1.00	33.08	471.99	0.84
22	4-undecyne	471.65	6	33.03	0.211	11	0	0	0	1.00	33.08	471.99	0.34
23	3-undecyne	473.15	6	33.24	0.298	11	0	0	0	1.00	33.17	472.64	0.51
24	2-undecyne	479.15	6	34.06	1.261	11	0	0	0	1.00	34.13	479.69	0.54
25	1-dodecyne	488.15	1	35.32	−0.324	12	0	0	0	1.00	35.32	488.21	0.06
26	4-dodecyne	492.15	2	35.89	0.211	12	0	0	0	1.00	35.86	491.94	0.21
27	5-dodecyne	492.15	2	35.89	0.211	12	0	0	0	1.00	35.86	491.94	0.21
28	3-dodecyne	492.55	6	35.95	0.298	12	0	0	0	1.00	35.95	492.55	0.00
29	2-dodecyne	499.15	6	36.91	1.261	12	0	0	0	1.00	36.91	499.15	0.00
30	1-tridecyne	507.15	1	38.10	−0.324	13	0	0	0	1.00	38.10	507.14	0.01
31	4-tridecyne	510.65	2	38.64	0.211	13	0	0	0	1.00	38.64	510.65	0.00
32	5-tridecyne	510.65	7	38.64	0.211	13	0	0	0	1.00	38.64	510.65	0.00
33	6-tridecyne	510.65	2	38.64	0.211	13	0	0	0	1.00	38.64	510.65	0.00
34	3-tridecyne	511.15	6	38.71	0.298	13	0	0	0	1.00	38.73	511.22	0.07
35	2-tridecyne	518.15	6	39.80	1.261	13	0	0	0	1.00	39.69	517.43	0.72
36	1-tetradecyne	525.15	1	40.91	−0.324	14	0	0	0	1.00	40.88	524.96	0.19
37	3-tetradecyne	528.45	2	41.45	0.298	14	0	0	0	1.00	41.50	528.80	0.35

*e-mail: quina@usp.br

Table S1. continuation

entry	compound	Lit. T_B/K	Ref.	Lit. Y_{BP}	A_i	C	M_3	M	D	S	Pred. Y_{BP}	Pred. T_B/K	AD/K
38	5-tetradecyne	528.55	2	41.46	0.211	14	0	0	0	1.00	41.42	528.26	0.29
39	6-tetradecyne	528.55	2	41.46	0.211	14	0	0	0	1.00	41.42	528.26	0.29
40	1-pentadecyne	541.15	1	43.55	−0.324	15	0	0	0	1.00	43.66	541.78	0.63
41	3-pentadecyne	544.15	6	44.07	0.298	15	0	0	0	1.00	44.28	545.42	1.27
42	2-pentadecyne	553.15	6	45.63	1.261	15	0	0	0	1.00	45.25	550.97	2.18
43	1-hexadecyne	557.45	2	46.39	−0.324	16	0	0	0	1.00	46.44	557.72	0.27
44	3-hexadecyne	559.15	6	46.70	0.298	16	0	0	0	1.00	47.06	561.17	2.02
45	2-hexadecyne	569.15	6	48.53	1.261	16	0	0	0	1.00	48.03	566.45	2.70
46	1-heptadecyne	572.45	2	49.14	−0.324	17	0	0	0	1.00	49.22	572.86	0.41
47	3-heptadecyne	573.15	6	49.27	0.298	17	0	0	0	1.00	49.84	576.15	3.00
48	2-heptadecyne	584.15	6	51.38	1.261	17	0	0	0	1.00	50.80	581.18	2.97
49	1-octadecyne	586.15	1	51.77	−0.324	18	0	0	0	1.00	52.00	587.29	1.14
50	3-octadecyne	587.15	6	51.97	0.298	18	0	0	0	1.00	52.62	590.43	3.28
51	2-octadecyne	598.15	6	54.18	1.261	18	0	0	0	1.00	53.58	595.23	2.92
52	1-nonadecyne	600.15	1	54.59	−0.324	19	0	0	0	1.00	54.78	601.07	0.92
53	3-nonadecyne	600.15	6	54.59	0.298	19	0	0	0	1.00	55.40	604.07	3.92
54	2-nonadecyne	612.15	6	57.10	1.261	19	0	0	0	1.00	56.36	608.66	3.49
55	1-icosyne	613.15	1	57.32	−0.324	20	0	0	0	1.00	57.56	614.25	1.10
56	2-icosyne	625.15	6	59.95	1.261	20	0	0	0	1.00	59.14	621.52	3.63
57	1-henicosyne	627.15	6	60.39	−0.324	21	0	0	0	1.00	60.34	626.89	0.26
58	1-docosyne	639.15	6	63.14	−0.324	22	0	0	0	1.00	63.11	639.02	0.13
59	1-tricosyne	651.15	6	66.00	−0.324	23	0	0	0	1.00	65.89	650.70	0.45
60	1-tetracosyne	662.15	6	68.73	−0.324	24	0	0	0	1.00	68.67	661.94	0.21
61	1-pentacosyne	672.15	6	71.29	−0.324	25	0	0	0	1.00	71.45	672.77	0.62
62	1-hexacosyne	682.15	6	73.94	−0.324	26	0	0	0	1.00	74.23	683.24	1.09
63	1-heptacosyne	692.15	6	76.67	−0.324	27	0	0	0	1.00	77.01	693.36	1.21
64	1-octacosyne	701.15	6	79.21	−0.324	28	0	0	0	1.00	79.79	703.15	2.00
65	1-nonacosyne	710.15	6	81.83	−0.324	29	0	0	0	1.00	82.57	712.63	2.48
66	1-triacontyne	719.15	6	84.53	−0.324	30	0	0	0	1.00	85.35	721.82	2.67
67	3-methyl-1-hexyne	358.15	5	20.37	−0.324	6	0	1	0	1.36	20.42	358.76	0.61
68	5-methyl-1-hexyne	360.15	4	20.55	−0.324	6	0	1	0	1.36	20.42	358.76	1.39
69	4-methyl-1-hexyne	364.15	6	20.92	−0.324	6	1	0	0	1.36	20.57	360.42	3.73
70	2-methyl-3-hexyne	368.35	6	21.31	0.298	6	0	1	0	1.36	21.04	365.49	2.86
71	4-methyl-2-hexyne	372.69	6	21.73	1.261	6	0	1	0	1.36	22.01	375.61	2.92
72	5-methyl-2-hexyne	375.61	6	22.01	1.261	6	0	1	0	1.36	22.01	375.61	0.00
73	6-methyl-3-heptyne	395.15	2	23.97	0.298	7	0	1	0	1.31	23.79	393.46	1.69
74	2-methyl-3-octyne	418.45	2	26.48	0.298	8	0	1	0	1.27	26.55	419.03	0.58
75	7-methyl-3-octyne	421.10	6	26.78	0.298	8	0	1	0	1.27	26.55	419.03	2.07
76	2,2,7-trimethyl-3-octyne	439.15	2	28.89	0.298	8	0	3	1	1.89	29.70	445.82	6.67
												AAD = 1.46 K	

Note: Because experimental data are not available, the data set does not include compounds with ethyl or propyl substituents, nor are there compounds with V, G, or T substitution patterns.

Table S2. Flash point data. All flash point (T_{FP}) and absolute deviation (AD) values have been rounded to the nearst tenth of a degree. Entry numbers are the same as in Table S1

entry	compound	Pred. Y_{BP}	Lit. T_{FP}/K	Ref.	Lit. N_{FP}	Pred. N_{FP}	Pred. T_{FP}/K	AD/K
1	1-hexyne	18.65	252.15	8	19.068	19.095	252.3	0.2
2	3-hexyne	19.27	259.15	5	20.113	19.709	256.5	2.7
3	2-hexyne	20.24	263.15	5	20.720	20.659	262.8	0.4
4	1-heptyne	21.43	271.15	8	21.953	21.838	270.4	0.7
5	3-heptyne	22.05	278.45	2	23.102	22.451	274.3	4.1
6	2-heptyne	23.01	281.15	2	23.533	23.402	280.3	0.8
7	1-octyne	24.21	289.15	5	24.826	24.581	287.6	1.5
8	4-octyne	24.74	291.15	5	25.154	25.108	290.9	0.3
9	3-octyne	24.83	295.15	2	25.813	25.194	291.4	3.8
10	2-octyne	25.79	297.25	2	26.162	26.145	297.1	0.1
11	1-nonyne	26.99	306.15	2	27.660	27.323	304.2	2.0
12	4-nonyne	27.52	311.45	2	28.567	27.851	307.3	4.2
13	3-nonyne	27.61	310.75	2	28.446	27.937	307.8	3.0
14	2-nonyne	28.57	312.15	2	28.687	28.888	313.3	1.2
15	1-decyne	29.77	321.15	8	30.254	30.066	320.1	1.1
16	4-decyne	30.30	325.45	2	31.014	30.594	323.1	2.4
18	3-decyne	30.39	325.35	2	30.996	30.680	323.6	1.8
19	2-decyne	31.35	326.09	2	31.128	31.631	328.9	2.8
20	1-undecyne	32.55	338.35	2	33.335	32.809	335.5	2.9
21	5-undecyne	33.08	338.75	2	33.408	33.337	338.4	0.4
22	4-undecyne	33.08	338.75	2	33.408	33.337	338.4	0.4
25	1-dodecyne	35.32	352.15	8	35.886	35.552	350.4	1.8
26	4-dodecyne	35.86	351.45	2	35.755	36.080	353.2	1.7
27	5-dodecyne	35.86	351.45	2	35.755	36.080	353.2	1.7
29	2-dodecyne	36.91	351.35	2	35.736	37.117	358.7	7.3
30	1-tridecyne	38.10	365.75	2	38.468	38.295	364.8	0.9
31	4-tridecyne	38.64	363.65	2	38.065	38.822	367.6	3.9
33	6-tridecyne	38.64	363.65	2	38.065	38.822	367.6	3.9
36	1-tetradecyne	40.88	378.15	5	40.880	41.038	379.0	0.8
37	3-tetradecyne	41.50	375.35	2	40.330	41.651	382.1	6.7
38	5-tetradecyne	41.42	375.35	2	40.330	41.565	381.6	6.3
39	6-tetradecyne	41.42	375.35	2	40.330	41.565	381.6	6.3
40	1-pentadecyne	43.66	390.15	5	43.265	43.781	392.7	2.6
67	3-methyl-1-hexyne	20.42	258.15	9	19.962	20.843	264.0	5.8
68	5-methyl-1-hexyne	20.42	266.15	9	21.179	20.843	264.0	2.2
73	6-methyl-3-heptyne	23.79	288.55	2	24.728	24.168	285.1	3.4
74	2-methyl-3-octyne	26.55	303.75	2	27.253	26.888	301.6	2.2
75	7-methyl-3-octyne	26.55	303.75	2	27.253	26.888	301.6	2.2
76	2,2,7-trimethyl-3-octyne	29.70	318.35	2	29.763	30.005	319.7	1.4
								AAD = 2.5 K

References

1. Driesbach, R. R.; *Physical Properties of Chemical Compounds.-II*, American Chemical Society: Washington, DC 1959.
2. http://www.lookchem.com accessed in September, 2012.
3. Brown, R. L.; Stein, S. E. In *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*; Linstrom, P. J.; Mallard, W.G., eds.; National Institute of Standards and Technology: Gaithersburg MD, http://webbook.nist.gov/chemistry/ accessed in September, 2012.
4. Ferris, S. W.08/13/2012 *Handbook of Hydrocarbons*, Academic Press: New York, 1955.
5. http://ull.chemistry.uakron.edu/erd accessed in September, 2012.
6. Yaws, C. L.; *Thermophysical Properties of Chemicals and Hydrocarbons*, William Andrew: Norwich, NY, 2008
7. http://www.guidechem.com/dictionary/en/60186-80-3.html accessed in September, 2012.
8. http://www.acros.com accessed in September, 2012.
9. http://www.sigmaaldrich.com accessed in September, 2012.